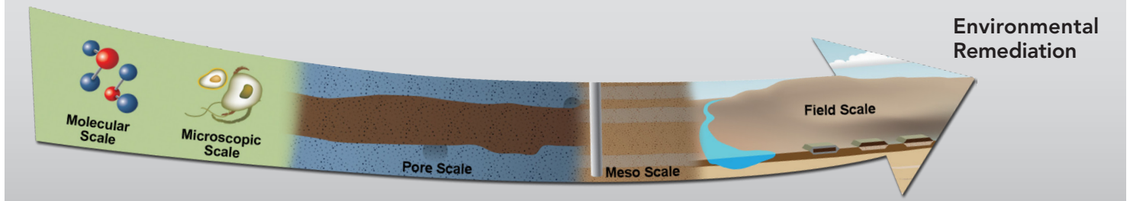
Seventeen major sites located across the United States were once used for nuclear material production, weapon development, and weapon testing. Several of these sites are now contaminated with radionuclides, metals, or hazardous chemicals. These contaminants create a significant environmental liability that the Department of Energy (DOE) is dedicated to cleaning up.

To date, DOE has made significant progress remediating these sites by embracing a mission based on reducing risk and reducing environmental liability through fundamental scientific understanding and applied technologies. DOE intends to accelerate this progress through the integrated efforts of its Office of Science (DOE-SC), and Office of Environmental Management (DOE-EM).



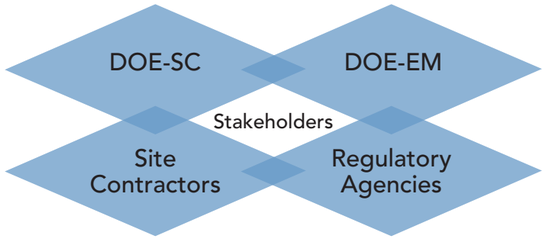
Approach

For DOE to successfully address remaining cleanup problems, it will require

- partnering and leveraging with other relevant organizations
- integrating basic science and "needs-driven" applied research activities with DOE cleanup operations to facilitate the transition of scientific results into applied solutions.

ASCEM will provide a technical basis for quantifying, and predicting, both natural and post-remediation contaminant discharge from the vadose zone to the groundwater. It will also facilitate the development of *in situ* solutions that limit contaminant discharge.

The knowledge gained through ASCEM will standardize performance and risk assessment across the DOE complex. ASCEM will also help transform fundamental science innovation into practical applications deployed by site contractors across the entire DOE complex.



Advanced Simulation Capability for Environmental Management (ASCEM)

ASCEM is being developed to provide a tool and approach to facilitate robust and standardized development of performance and risk assessments for cleanup and closure activities throughout the EM complex.

The ASCEM team is composed of scientists from eight National Laboratories. This team is leveraging Department of Energy (DOE) investments in basic science and applied research including high performance computing codes developed through the Advanced Scientific Computing Research and Advanced Simulation & Computing programs as well as collaborating with the Offices of Science, Fossil Energy, and Nuclear Energy.

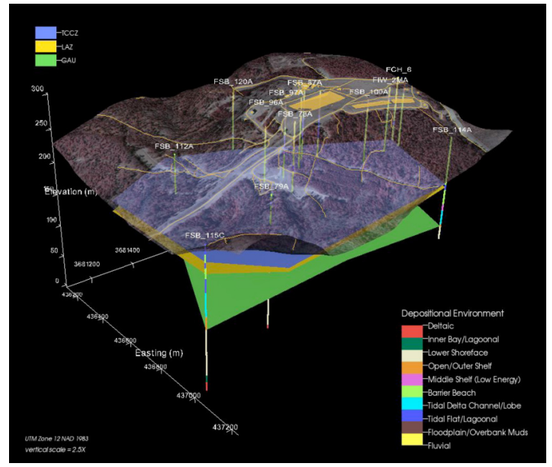
Challenge

Current groundwater and soil remediation challenges that will continue to be addressed in the next decade include cost-effective characterization, remediation, and monitoring of contaminants in the vadose zone and groundwater. Many of the contaminated sites in the EM complex require additional characterization, most require final remediation decisions, and all of them will require long-term monitoring.

To address these remediation requirements, the EM office of Technology Innovation and Development, Groundwater and Soil Remediation (EM-32) began the program Advanced Simulation Capability for Environmental Management (ASCEM). ASCEM is a state-of-the-art scientific tool and approach for integrating data and scientific understanding to enable prediction of contaminant fate and transport in natural and engineered systems. This initiative supports the reduction of uncertainties and risks associated with DOE EM's environmental cleanup and closure programs by better understanding and quantifying the subsurface flow and contaminant transport behavior in complex geological systems. This includes the long-term performance of engineered components, including cementitious materials in nuclear waste disposal facilities that may be sources for future contamination of the subsurface.

To support economically sound and sustainable solutions, ASCEM will:

- Provide predictive capabilities for fate and transport of contaminants.
- Provide an integrated set of tools for advanced visualization, data manipulation, and uncertainty quantification to aid in decision making.
- Allow for advanced modeling of proposed remedial activities.



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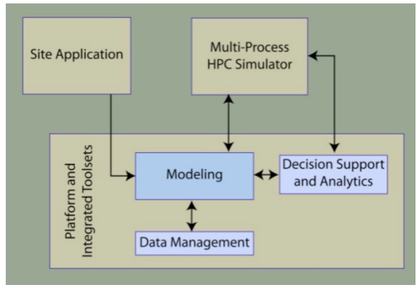
The mission of ASCEM is to develop a modular and extensible open-source, high performance computing (HPC) modeling system for multiphase, multicomponent, multiscale subsurface flow and contaminant transport, and source-term degradation, enabling robust and standardized future performance and risk assessments for EM cleanup and closure activities.

ASCEM

Advanced Simulation Capability for Environmental Management

ASCEM Thrust Areas

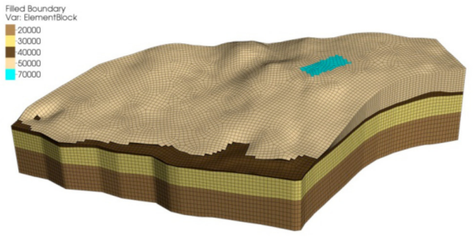
- High Performance Computing
- Platform and Integrated Toolsets
- Site Applications



High Performance Computing

The ASCEM computational engine, Amanzi, will allow for reactive flow and transport on both structured and unstructured grids, and include physical process such as:

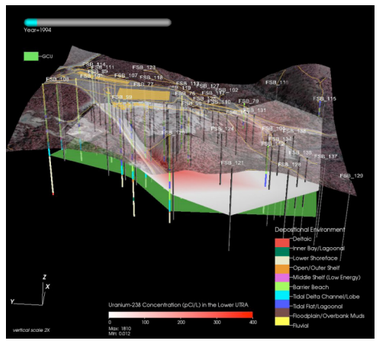
- Biochemical Reaction Processes
- Transport of Colloids
- Thermal Effects
- Mechanical Effects, and
- Cementitious Source Term Degradation



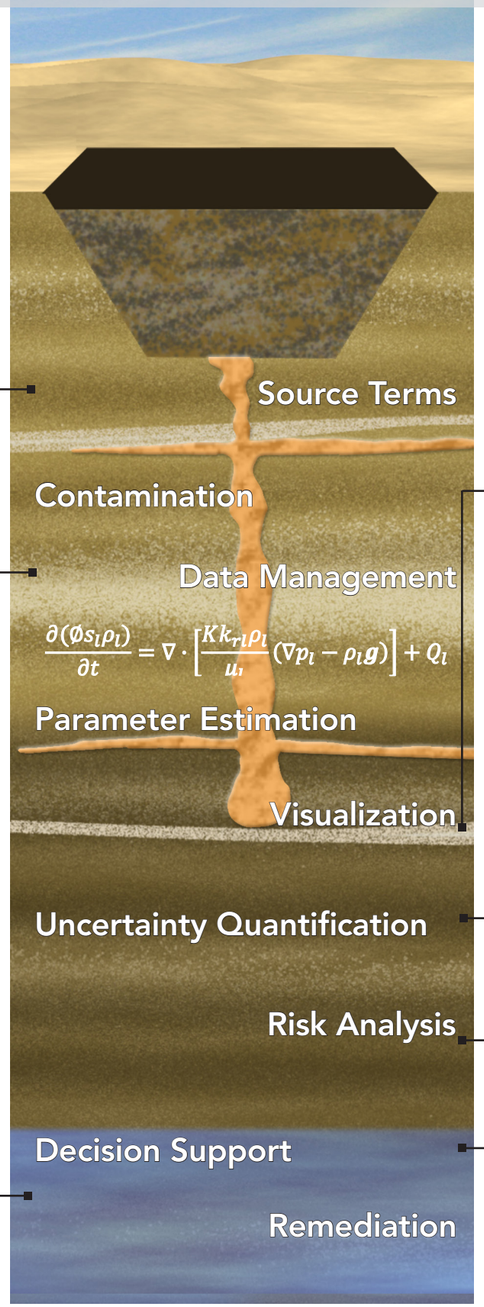
Platform and Integrated Toolsets

ASCEM will include toolsets for:

- Model Setup
- Data Management
- Visualization
- Uncertainty Quantification
- Parameter Estimation
- Decision Support
- Risk Analysis

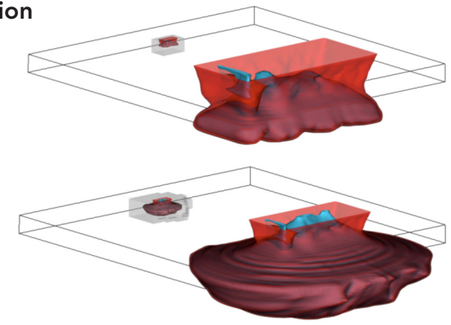


These tools will allow users to quickly and efficiently create and analyze simulation data assisting highlighting relevant processes and parameters allowing for informed decision making.



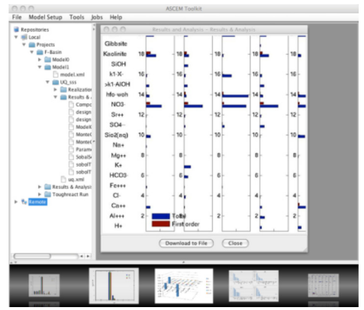
Capability Highlight: Visualization

Advanced Visualization will not only allow users to view data in 2 and 3 dimensions and with movies, but it will also help users pick the most relevant data to view. This toolset will allow users to view historic data as well as simulation results in an interactive manner.



Capability Highlight: Uncertainty Quantification

The uncertainty quantification toolset will propagate input variations and uncertainties through the forward model. In models where this technique is computationally restricted, the toolset will provide methodologies to maximize the benefit from a limited number of forward model runs.



Site Applications

The Site Applications thrust area provides the main link between ASCEM and the EM community's modeling and regulatory needs; it is vital to ensuring that ASCEM HPC modeling capabilities are widely accepted across the EM Complex. This thrust incorporates a "user interface" task focused on establishing contact with end users, soliciting their input about ASCEM development plans, and conveying the feedback to members of the HPC and Platform Thrust areas responsible for the tool and code development.

Providing Scientific and Technical Defense for Waste management and Remedial Actions

Working with the Applied Field Research Initiatives, ASCEM will provide predictions of contaminant fate and transport that will allow better defense of regulatory decisions. Users will be able to determine the rigor and complexity of modeling and apply them in a graded approach whether simple or complex models are used. This will lead to development of better remedial and waste management actions and reduction in development times and cost-effective clear-up technologies and waste management approaches.

Berkeley Lab · Los Alamos National Laboratory · Pacific Northwest National Laboratory · Oak Ridge National Laboratory · SRNL Savannah River National Laboratory · Lawrence Livermore National Laboratory · Argonne National Laboratory · INL Idaho National Laboratory